

Keynote Forum May 13, 2019

Chemistry 2019



9th World Congress on

Chemistry and Medicinal Chemistry

May 13-14, 2019 | Prague, Czech Republic



Chemistry and Medicinal Chemistry

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Andrés E Dulcey

National Institute of Health, USA

Discovery, optimization and characterization of CNS-Penetrant Allosteric Inhibitors of c-Abl Kinase

he loss of different neuronal populations leading to neuronal dysfunction, cytoskeletal alterations and abnormal protein phosphorylation are the main hallmarks of neurodegenerative diseases. In particular, the neuropathological hallmarks of Alzheimer's disease (AD) are neuronal loss in regions related to memory and cognition, neurotransmitter depletion, synaptic alteration and the deposition of abnormal protein aggregates. Currently, there is no effective treatment for AD, creating a need for new therapeutic treatments that can treat or prevent AD and other neurodegenerative diseases. c-Abl tyrosine kinase is a ubiquitous non-receptor tyrosine kinase involved in signal transduction. In addition to its classic function in leukemia pathogenesis, c-Abl is also thought to play a role in neuronal development, neurogenesis, neuronal migration, axonal extension, and synaptic plasticity, whereby deregulation of c-Abl could be related to early neuronal dysfunction and cytoskeletal alterations. Here we describe the chemical and pharmacological characterization of novel brain-penetrant allosteric inhibitors of c-Abl tyrosine kinase activity, with

proof of principle towards their applicability as a potential treatment for neurodegenerative disorders.

Speaker Biography

Andrés E Dulcey was born in Cali, Colombia. After completing a Bachelor of Science in Chemistry from the Ohio State University, he joined the laboratory of Professor Virgil Percec at the University of Pennsylvania. His doctoral research focused on the design, synthesis and structural characterization of biologically-inspired libraries of amphiphilic compounds which self-assemble into functional, helical, porous channels. After completion of his doctoral degree, he joined the National Institutes of Health (NIH), first as a Postdoctoral Fellow and then as a Research Scientist, where he has spent over 10 years working in different modalities of medicinal chemistry. Currently, he is at the National center for advancing translational sciences at the NIH, where he works as a Research Scientist at the forefront of translation, advancing programs in target identification and validation, assay development and screening, probe development and lead optimization, and drug repurposing, with the goal of furthering the understanding of biochemical pathways and aiding the development of new medicines.

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Igor V Alabugin

Florida State University, USA

From Alkyne Origami and Metal-Free C-H aminations to electron upconversion: An array of new bottom-up approaches to Carbon-rich molecules and materials

This talk will outline new strategies for assembling carbonrich conjugated structures. In the 1st part, I present alkynes as unique high-energy synthetic precursors for extended polyaromatics, the two general patterns of oligoalkyne folding into a graphenic ribbons, and the use of supramolecular effects in the design of radical cascades.

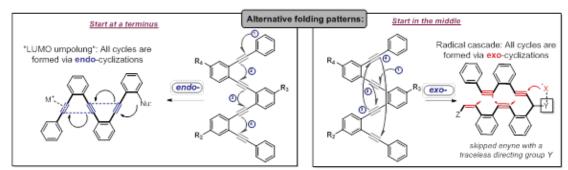
In the 2^{nd} part, I will present a mild method for oxidative C-H amination from unprotected anilines and C(sp³)-H bonds. In this process, basic, radical, and oxidizing species work together in a coordinated sequence of deprotonation, H-atom transfer and electron transfer that forges a new C–N bond in a conceptually unique manner. This approach leads to efficient assembly of extended N-doped helicenes.

I will also introduce reductant upconversion, a new concept in catalysis, and show how it can be used to achieve the precise timing of oxidation steps in reaction cascades.

Speaker Biography

Igor V Alabugin received his Ph.D. degree from Moscow State University, Russia. After a postdoctoral study at the University of Wisconsin-Madison, he joined the Florida State University, Department of Chemistry and Biochemistry in 2000, where he is currently the Cottrell Professor. His efforts in the development of new reactions for selective DNA cleavage in cancer cells, bioorthogonal chemistry, functionalization of nanomaterials, and construction of graphene ribbons are greatly assisted by fundamental studies of stereoelectronic effects. He has published over 150 peer-reviewed research articles and a book on stereoelectronic effects. He has also given ~200 talks at conferences, universities and industries. He also serves on the editorial board of three journals. His recent awards include selection as an AAAS Fellow 2017 and Fulbright Fellow (2018).

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Shaodong Guo

Texas A&M University, USA

Phytochemicals and Dietary Intervention in control of Diabetes, Obesity and CVD

he growing prevalence of metabolic syndrome (MetS) in the US and even worldwide is becoming a serious health problem and economic burden. MetS has become a crucial risk factor for the development of Type 2 Diabetes Mellitus (T2D) and Cardiovascular Diseases (CVD). In this seminar, we discuss mechanisms of MetS pathogenesis and phytochemical role from tea in control of glucose homeostasis focusing on the Forkhead/winged helix transcription factor O-class member 1 (FoxO1), a key mediator of insulin and glucagon signaling in control of glucose homeostasis. One of the most potent phytochemicals from tea is epigallocatechin gallate (EGCG) that has been attracted interests owing to its potential to combat hyperglycemic diabetes, but molecular mechanisms underlying its antihyperglycemic effect, in particular the effect on FoxO1 is poorly understand. This study aims to assess the impact of EGCG on the glucagon signaling pathway in regulating glucose metabolism. A novel mechanism of EGCG in restraining Hepatic Glucose Production (HGP) is through antagonizing glucagon signaling and Foxo1. EGCG may serve as a promising compound for regulating glucose homeostasis and benefit to CVD.

Speaker Biography

Shaodong Guo is Associate Professor in the Department of Nutrition and Food Science at Texas A&M University College. He received his Ph. D in Physiology from Peking University, China. Then he completed his postdoctoral research training in Genetics, Biochemistry, and Medicine in the Chinese Academy of Sciences, the University of Illinois at Chicago, and Harvard University, respectively. He was Instructor in Medicine at Children's Hospital Boston and Harvard Medical School for two years prior to joining the faculty at Texas A&M Health Science Center. Currently, He serves as senior editor for the Journal of Endocrinology and Journal of Molecular Endocrinology, two major official journals of Endocrine Society of Europe, UK, and Australia, and he is the textbook chapter writer for Metabolic Syndrome edited by Rexford Ahima and published by Springer in 2016. His lab research focuses on insulin/ glucagon and estrogen signal transduction, insulin resistance, gene transcriptional control of nutrient homeostasis, and cardiac dysfunction in diabetes. He has been working on the gene transcriptional regulation of metabolic homeostasis by insulin receptor substrate proteins (IRS) and Forkhead FoxO transcription factors and he has been funded by American Diabetes Association (ADA), American Heart Association, and the National Institute of Health of USA. He is a recipient of ADA junior faculty award, career development award, and Richard R Lee Research Excellence Award. His work has been published in a number of journals including the JBC, Endocrinology, Hypertension, Diabetes, Circulation Research, AJP, MCB, and Nature Medicine, receiving more than 5,500 citations from the Google Scholar.

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Martin C Feiters

Radboud University, The Netherlands

Cationic gemini and geminoid peptide amphiphiles: From transfection to Protease inhibition

Gemini surfactants are amphiphilic molecules containing two head groups and two aliphatic tails which are linked by a spacer between the head groups, or between the linker region connecting the heads and the tails. Because their critical aggregate concentration is 10^3 -fold lower they are more effective surfactants than the corresponding monovalent compounds (*i.e.* classical surfactants with a single chain and a single head group), which makes them interesting for various biomedical applications.

Cationic geminis have shown to be viable agents for transfection, the introduction of nucleotides into a eukaryotic cell, thereby providing an alternative to viruses and cationic polymers. Amphiphilic peptides consisting of a peptide spacer with the N- and C-termini appended with hydrophobic groups are asymmetric geminis and are called gemini-like or geminoids. Interestingly, the SPKR geminoid with unsaturated alkyl tails can achieve transfection without the lysogenic helper lipid that is required in other cases.

The proteases involved in the maturation of the polyprotein of dengue virus to new virus particles have cationic peptide sequences as their preferred substrates. Saturated geminoids of the KG_nK and KA_nK series (n = 1 or 2) are inhibitors of dengue virus 2 protease and the

host protease furin, with slight selectivity of one over the other.The inhibitors are also active against dengue virus 2 infection in a cellular context, at concentrations below which they are toxic.

Speaker Biography

Martin C Feiters graduated in biochemistry, bio-organic chemistry and food chemistry and did PhD research on structure-function relationship of the enzyme lipoxygenase, followed by postdoctoral work in X-ray absorption spectroscopy, before his appointment as Associate Professor at Radboud University (1989). He has > 150 publications and a number of patents. He has applied various kinds of radiation, viz. synchrotron X-rays and neutrons, to the elucidation of supramolecular structures such as viruses, lipid-DNA complexes, and porphyrin assemblies, as well as the coordination chemistry of metals in homogeneous catalysts, metalloproteins, and biological non-metal trace elements such as bromine and iodine. He has contributed to the development of hyperpolarization in NMR, viz. by the optimization of the catalyst and the co-substrate approach for detection and quantitative analysis by Signal Amplification by Reversible Exchange (SABRE) and high-field non-hydrogenative para-hydrogen-induced hyperpolarization (PHIP) at micromolar concentrations. He is involved in the developments of various drugs, viz. antimalarials, cyclodextrinbased steroid transporters, and amphiphilic peptides for transfection as well as, together with his spin-off company Protinhi Therapeutics, as inhibitors of viral proteases.

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Qi Zhang Biaolin Peng

Cranfield University, UK

Giant electrocaloric effect found in the relaxor PLZST thin films with the coexistence of antiferroelectric and ferroelectric phases in a broad temperature range

arge electrocaloric (EC) effect with a broad operational temperature range is required and attractive in solid-state cooling devices. In this work, a giant EC effect (ΔT~20.7K) in a broad temperature range (~ 110 K) was demonstrated in relaxor antiferroelectric (AFE) $Pb_{0.97}La_{0.02}(Zr_{0.65}Sn_{0.3}Ti_{0.05}) O_3$ (PLZST) sol-gel thin film. The use of the LaNiO₂/Pt composite bottom electrode may cause the in-plane residual thermal tensile stress during the layer-by-layer annealing process, which may be responsible for the large positive EC effect. The coexistence of nanoscale multiple FE and AFE phases leads to the great dielectric relaxor dispersion around the dielectric peak, which may be ascribed to the broad EC operational temperature range. These newly-discovered properties in the PLZST thin films suggest this multifunctional material having a great potential for applications in modern solid-state cooling.

Speaker Biography

Qi Zhang is a senior lecturer in Cranfield University, UK and a professor in Wuhan University of Technology, Wuhan, China. He has his expertise in functional materials. He was one of the initiators of the thin film electrocaloric effect, which could develop. He has authored or coauthored over 200 papers, edited one book and 10 book chapters. He has an h factor of 30. He is a fellow and charted scientist in IOM3. His main areas of research are within synthesis of nanomaterials for electrochemical energy storage, fabrication of transparent conducting thin films and sol-gel synthesis and structural characterization of ferroelectric thin films for electrocaloric cooling. He was the recipient of the Royal Society Brian Mercer Feasibility Award.

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Loredana De Bartolo S Morelli, A Piscioneri, S Salerno, L Giorno and E Drioli

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Polymeric membrane platform for testing the neuroprotective effect of molecules in Alzheimer's disease

wide range of polymeric membranes have been synthesised for creating suitable biomaterials to provide topographic, chemotactic, and haptotactic cues to improve neuronal regeneration. Polymeric membranes thanks to their selective structural, physico-chemical, mechanical and transport properties, are able to drive neurite outgrowth and branching, network connectivity, and synaptic plasticity leading to the successful in vitro reconstruction of neuronal tissue. Indeed, membranes can be employed to create an in vitro neuronal tissue model for studying neurobiological events, for pharmacological screening, and as investigational platforms for neurodegenerative diseases. Within this scenario, the approach was to synthesize microporous polymer membranes combining the intrinsic properties of the polymer as well as the geometry and configuration of the membranes with the perfusion conditions of a bioreactor, in order to develop a well-controlled microenvironment able to trigger neuronal differentiation. The selective permeability of the membranes and the optimized fluid dynamic conditions created by the membrane bioreactor provide a 3D low-shear stress environment fully controlled at molecular level with enhanced diffusion of nutrients and waste removal that successfully develops neuronal-like tissue. The membrane platform was used to reproduce an in vitro model of Amyloid beta (Abeta)-induced toxicity associated to Alzheimer's

Notes:

disease to test the neuroprotective effect of molecules such as crocin and glycitein. Using this approach, we showed the neuroprotection of the administered molecules that inhibit the cytotoxic event triggered by β -amyloid while maintaining high cell viability, reduces the number of cells in apoptosis by inactivating specific protein markers and protects against ROS production by highlighting an antioxidant action. Thus, the membrane is an innovative investigational platform that could be used to study neurodegenerative disorders as well as neurobiological phenomena in order to gain new insights on neurological functions and protection.

Speaker Biography

Loredana De Bartolo, PhD. in Chemical Technologies and New Materials, is research director at the Institute on Membrane Technology of the National Research Council of Italy (ITM-CNR). Her research expertise is in the field of membrane bioartificial organs, membrane bioreactors, membrane separation processes in life science. She is scientific responsible of several European, national and international projects. She is involved in several international committees and in editorial board of prestigious scientific journals. She is author of over 150 papers published in international journals/books and encyclopaedia and has made numerous invited and keynote lectures to scientific meetings. She was named International Fellow in World Federation on Preventive and Regenerative Medicine and Alexander von Humboldt Fellow.

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György Keglevich

Budapest University of Technology and Economics, Hungary

Microwave irradiation and catalysis in Organophosphorus Chemistry– Green Synthesis of biologically active Organophosphorus Compounds

'he microwave (MW) technique has become an important tool in organophosphorus chemistry [1-3]. In this paper, the advantages of MWs in different catalytic reactions are surveyed. The first case is, when the MW-assisted direct esterification of phosphinic acids becomes more efficient in the presence of an ionic liquid catalyst. The second instance is, when catalytic reactions, such as the phase transfer catalyzed (PTC) O-alkylation of phosphinic acids, or the Arbuzov reaction of aryl bromides are promoted further by MW irradiation. It is also an option that MWs may substitute catalysts, such as in the PTC alkylation of active methylene containing P-derivatives, in Kabachnik-Fields condensations, and in reluctant P=O deoxygenations. Another valuable finding of ours is that in the Hirao P-C coupling applying Pd(OAc), as the catalyst, the slight excess of the >P(O)H reagent may substitute the usual P-ligands. It is also the purpose of this paper to elucidate the scope and limitations of the MW tool, to interpret the special MW effects, and to model the distribution and effect of the local overheatings. All these considerations were possible on the basis of the results of our quantum chemical calculations and utilizing

the pseudo first order kinetic equation and the Arrhenius equation. The synthesis of dronic acid derivatives as drugs in the therapy of bone diseases is also discussed.

Speaker Biography

György Keglevich graduated from the Technical University of Budapest in 1981 as a chemical engineer. He got "Doctor of Chemical Science" degree in 1994, in the subject of organophosphorus-chemistry. He has been the Head of the Department of Organic Chemistry and Technology since 1999. Within organophosphorus chemistry, his major field embraces a P-heterocycles involving selective syntheses, as well as bioactive and industrial aspects. He also deals with environmentally friendly chemistry involving MW chemistry, its theoretical aspects, phase transfer catalysis, the development of new chiral catalysts, and the use of ionic liquids. He is the author or co-author of ca. 550 papers (the majority of which appeared in international journals) including ca. 70 review articles and 40 book chapters. He is, among others, the member of the Editorial Board of Molecules, Heteroatom Chemistry and Phosphorus, Sulfur and Silicon, and the Related Elements, and Current Microwave Chemistry. He is the Editor-in-Chief for Current Organic Chemistry and Current Green Chemistry, the co-Editor-in-Chief for Current Catalysis, Associate Editor for Current Organic Synthesis and Letters in Drug Design and Discovery, and Regional Editor for Letters in Organic Chemistry.

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María-Paz Zorzano

National Institute of Aerospace Technology, Spain

Hydrogen chemistry in Space Exploration: In-situ resource utilization

Ithough hydrogen is the most common element on Athe universe, having access to large amounts of it in space and transforming it in a way that it can be useful for exploration is a challenge. The development of in-situ resource-utilization (ISRU) methods for space exploration is a new research activity which is being supported both by NASA and ESA. The Exploration Roadmap of ESA and NASA to fulfil: 1) the Human and Robotic exploration of the Moon; 2) the Deep Space Gateway and 3) the human exploration of Mars has been defined, and the first steps are now being implemented. However, the requirements on propellant mass do not allow for large landed missions. The future Mars Ascent Vehicle for humans will require about 7.0 mT of methane and 22.7 mT of oxygen to liftoff from Mars, back to Earth, with 4 crew members. This represents about 80% of the weight of the spacecraft, and this is to date one of the most critical problems that inhibits the human exploration of Mars. Methane, CH, has been observed on the Martian surface by the Curiosity rover, however only at trace-amount levels. The chemistry of methane production and destruction on Mars is to date not understood. New emerging space companies as SpaceX have declared their intention to investigate propellant production for Mars exploration. In addition to propellants, such as CH₄, water, H₂O, is another critical product, both for life- support systems and for its possible transformation into hydrogen, H₂, and oxygen, O₂, for propulsion or again

for life-support systems. In this talk we will review where are the main sources of hydrogen in the form of water on Mars and the Moon and how can this water be captured and transformed to facilitate the human and robotic exploration of space. We will review a few options for the sustainable production of methane on Mars, and the ISRU concentration and purification of water. Some of these processes may also have an industrial application on Earth.

Speaker Biography

María-Paz Zorzano is a researcher at the Centro de Astrobiología (CAB), of the National Institute of Aerospace Technology (INTA, Spain) and a Professor in Atmospheric Science at the Luleå University of Technology (LTU, Sweden). She is a planetary physicist, investigating space exploration and astrobiology. She is involved in multiple NASA and ESA missions of exploration of the Earth, Moon and Mars, including the Curiosity rover of the Mars Science Laboratory mission (NASA), the Exomars Trace Gas Orbiter (ESA), the ExoMars Rover (ESA) and the ExoMars Surface Platform (Roscosmos / ESA), as well as on proposals for the future international exploration of the Moon through the ESA Moon landers missions or the Deep Space Gateway. She is member of the COSPAR Planetary Protection Panel. She has received multiple awards related to space, such as the 2018 finalist award of the Space Exploration Masters Challenge and 2nd prize of the InnoSpace Masters call of 2018. She was also awarded in 2013 with a NASA Group Achievement for her contributions to the instrument REMS on board the Curiosity Rover. She is author of 85 refereed articles and several book chapters.

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Simona Collina Marta Rui, Giacomo Rossino and Daniela Rossi

University of Pavia, Italy

Across the "Universe" of Sigma receptor modulators. The experience of the MedChemLab

Cigma Receptors (SRs) represent an interesting orphan Oclass of molecular targets to hit for counteracting neurodegenerative diseases and cancer. They can be divided into two receptor subtypes (S1R and S2R, respectively), endowed with different physio-pathological and structural properties. From a therapeutic standpoint, the pharmacological activity of S1Rs is strictly related to the modulators that they interact with. In detail, S1R agonists promote neuroprotection and neuroplasticity, whereas antagonists can be beneficial in thwarting neuropathic pain and tumorous manifestations. Conversely, S2R modulators may have a pivotal role as anticancer agents. So far, four compounds reached the Clinical Stage of the Drug Discovery Process, as drug candidate in therapy and diagnosis for Alzheimer's disease (ANAVEX 2-73, AVP-923), for neuropathic pain (MR309) and cancer ([18F]-ISO-1).

The Medicinal Chemistry Laboratory (MedChemLab) is part of this scenario and has a long lasting experience in this field. Indeed, the group spent its efforts in designing and synthetizing molecules with affinity and selectivity towards SRs and discoved (R)-RC-33 and RC-106 as promising compounds. (R)-

RC-33 is a S1R agonist compound, characterized by good S1R affinity, good in vivo pharmacokinetic profile and endowed with neuroprotective properties. RC-106 is a pan-SR ligand (S1R antagonist and S2R agonist) showing anticancer activity towards a panel of cancer cell lines. These encouraging results lead members of the MedChemLab group to keep believing that SR modulators could become a relevant opportunity in the pharmaceutical field. Accordingly, throughout this speech the state-of-art and new insights of SRs, as well as the MedChemLab projects will be depicted.

Speaker Biography

Simona Collina is interested in the design and synthesis of small molecules, peptides, and peptidomimetics, focusing on their therapeutic application, in particular in neurodegenerative diseases, cancer and pain. Her interests also focus on drug discovery from natural sources. Among the different research topics, the discovery of small molecules able to affect the protein kinase C (PKC)/ELAV proteins/ mRNA system as well as new modulators of sigma receptors as well as of are the most challenging.

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Stergios Pispas

National Hellenic Research Foundation, Greece

Cationic block copolymer based nanocarriers for Proteins and Nucleic Acids

ne of the goals of polymeric nanomedicine is the creation of functional nanocarriers for pharmaceutical compounds taking advantage of developments in polymer synthesis and control over polymer self-assembly. The aim of this presentation is to discuss block copolymer based advanced nanocarriers for insulin and nucleic acids. We have utilized several novel cationic block polyelectrolytes for complexation with insulin and DNA/RNA as well block copolymer micelles encapsulating magnetic iron oxide nanoparticles for introducing multifunctionality in our polymer based nanocarriers. Static, dynamic and electrophoretic light scattering techniques and transmission electron microscopy were used in order to extract information on the size, charge and morphological characteristics of the nanostructures. Cytotoxicity, internalization into cells and gene transfection studies were also performed in the case of DNA/RNA carriers. Toxicity of nanocarrier systems was low. Application

of a magnetic field improved gene transfection in cell lines investigated.

Speaker Biography

Stergios Pispas is Director of Research at TPCI-NHRF. He serves as the chairman of the Scientific Council of TPCI-NHRF (since 2016) and an Advisory Board Member of the European Polymer Journal (2017) among other editorial duties. He has been awarded the American Institute of Chemists Foundation Award for Outstanding Post-doctoral Fellow (1995) and the A. K. Doolittle Award of the American Chemical Society (2003). He is a coauthor of more than 300 research articles in referred journals, several invited review articles and three books, receiving more than 7500 citations (h-index=40). His current research focuses on the synthesis of functional block copolymers by controlled polymerizations and the development of complex, hybrid, self-organized nanostructures based on designed synthetic polymers and biomacromolecules and inorganic nanomaterials for nanomedicine applications.

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Mineo Hiramatsu

Meijo University, Japan

3D graphene network as catalyst support material for electrochemical applications

raphene-based materials have attracted much Gattention due to their outstanding properties as well as emerging applications. Carbon nanowalls (CNWs) are fewlayer graphenes standing vertically on a substrate forming a self-supported network of 3-dimensional wall structures. CNWs and similar vertical graphene structures are sometimes decorated with metal nanoparticles. The mazelike architecture of CNWs with large-surface-area graphene planes would be useful as electrodes for energy devices and electrochemical sensors. CNWs can be synthesized by plasma enhanced chemical vapor deposition (PECVD) techniques on heated substrates (600-750 °C) employing methane and hydrogen mixtures. The height of CNWs increases almost linearly with the growth period, while the thickness of walls and interspaces between adjacent walls are almost constant. We have carried out CNW growth using PECVD, and the surface of CNWs was decorated with Pt nanoparticles by the reduction of chloroplatinic acid or by the metal-organic chemical deposition employing supercritical fluid. We report the performances of fuel

cell and hydrogen peroxide sensor, where CNW electrode was used. From the electrochemical evaluation, it was confirmed that Pt-supported CNWs had seven times higher durability than the conventional carbon black. In the case of hydrogen peroxide sensing, amperometric response results indicated that the Pt-decorated CNWs exhibited a wide linear range of 10–1500 μ M. Electrochemical experiments demonstrate that CNWs offer great promise for providing a new class of nanostructured electrodes for fuel cell and electrochemical applications.

Speaker Biography

Mineo Hiramatsu is a Full Professor of Department of Electrical and Electronic Engineering and the Director of Research Institute, Meijo University, Japan. His main fields of research are plasma diagnostics and plasma processing for the synthesis of thin films and nanostructured materials. He served as chairman and member of organizing and scientific committees of international conferences on plasma chemistry and plasma processing. He was awarded the Japan Society of Applied Physics Fellow in 2017.

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Zongwei Xu¹ Mathias Rommel²

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P-type 4H-SiC by Al Implantation and subsequent Annealing -Simulation, characterization and device design development

P-type doped 4H-SiC with very low resistivity is still one challenging technology in semiconducting fields. It is well accepted that p-type doping of 4H silicon carbide (SiC) by Al implantation and subsequent annealing results in free charge carrier concentrations which are significantly below what would be expected from activated and ionized Al concentrations. This is commonly explained by so-called compensating defects induced during the implantation process and which remain after annealing. Here, the experimentally determined compensation ratio (i.e., the ratio of defect concentration to activated Al concentration) is increasing with decreasing Al concentration. Obviously, this compensation significantly hinders the fabrication of todays and future SiC electron devices where both, fabrication of regions with moderate p-doping concentrations (such as p-well regions or junction determination structures) where accurate concentrations are required as well as regions where very high doping concentrations (e.g., ohmic contacts) are required.

In this talk, Molecular Dynamics (MD) simulations, Raman spectroscopy and sheet resistance measurements were used to study the preparation processes of low-resistance p-type 4H-SiC by Al ion implantation with ion doses of 2.45×10^{12} - 9.0×10^{14} cm⁻² and annealing treatment with temperatures of 1700 - 1900 °C. Greatly different from the LOPC (longitudinal optical phonon-plasmon coupled) Raman mode found from the sample of doping 4H-SiC during epitaxial growth, no significant influence on the surface concentration could be found for the longitudinal optical (LO) mode of Al-implanted 4H-SiC samples. When the Al surface concentration is larger than around 1018 cm⁻³, it was found that the intensity of the LO+ Raman peak (~ 980 - 1000 cm₋₁) increases and its full width

at half maximum (FWHM) drops with the increase of surface concentration after annealing treatment. Moreover, for surface concentrations above 10^{18} cm⁻³, the LO+ Raman peak showed a left shift towards the LO peak, which could be related to the increase of free carrier concentration in the Al-implanted 4H-SiC samples. After higher annealing temperatures of 1800 °C and 1900 °C, the crystallinity of Al-implanted 4H-SiC was found to be improved compared to annealing at 1700 °C for surface concentrations larger than 10^{18} cm⁻³, which is consistent with the results of sheet resistance measurements.

Speaker Biography

Zongwei Xu, Dr. Engineering, has his expertise in Micro/nano Manufacturing and Metrology. He was one of the pioneers of Micro/ nano Functional Structures Fabricated using Ion Beam Machining. He has illustrated the Multi-parameters' Coupling Mechanism involved in nanoscale effects and developed several methodologies using Ion Beam Nanofabrication. Several functional structures, including Siemens Star Metrology template and Photomask Template in nanolithography, have been developed and applied in Erlangen-Nuremberg University, Germany, Mitutoyo Research Center Europe and Chinese Academy of Sciences. More recently, he has conducted Activation of 4H-SiC p-type Doping by Al Implantation and Subsequent Annealing - Simulation, Characterization and Device Design Development. He is author of over 60 papers, 6 book chapters on Micro/nano Manufacturing and owner of 12 patents. He was the recipient of several Awards, including "Newton Fund" granted by the Royal Society, "Young Researchers" Awards (the 14th China-Japan International Conference on Ultra-Precision Machining Process (CJUMP2018), and the 3rd Asian Precision Engineering and Nanotechnology International Conference (ASPEN2009)). He was the Associate Editor of Journal of Mechanical Engineering Science, Guest Editor of Current Nanoscience, and the Editorial Board Member of three International Journals.

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Adriany Amorim

Earth University, Costa Rica

Extraction and development of Natural Products as an alternative strategy for disease control

Inflammation consists of an answer of the organism, triggered by different types of injuries on the tissues or for infectious agents. Although inflammatory answer is considered a protective event, pro-inflammatory mechanisms may contribute to the development of chronic diseases, such as diabetes, cancer, arthritis, neurological diseases and psoriasis, which is why the control of the inflammatory process is desired.

Many researches have focused on new bioactive molecules, natural products and functional foods as alternatives to the development of new anti-inflammatory agents. Several studies have also demonstrated the neuroprotective, hepatoprotective, cardioprotective, antifungal, anti-inflammatory, and anticancer activities of natural compounds as lycopene.

Furthermore, lycopene pretreatment at various doses significantly delayed tumor formation and growth, thereby reducing skin carcinogenesis in female ICR mice. Generally, lycopene inhibits cell proliferation, arrests cell cycle in different phases, and increases apoptosis in breast, colon, and prostate cancer lines. Therefore, the idea behind this conversation will be talking about some compounds extracted from food with activities anti-inflammatory and antioxidant, which work singly or in an association, might influence in the inflammatory process, reducing its harmful effects and the risk to develop diseases as breast cancer.

Speaker Biography

Adriany Amorim, Ph.D. in Biotechnology, is Industrial chemistry since 2002 and PhD in Biotechnology from Federal University of Piauí - Brazil in 2015 and from Autonomous University of Madrid - Spain in 2017. She has expertise in the extraction of antioxidants and developed an extraction process of natural antioxidant by clean technology. Therefore, she published two patents on this subject, one in Brazil and another in Portugal. In her last publications on medicinal chemistry, she has shown the effect of lycopene, extracted from natural source, against human breast adenocarcinoma cell and, its effects on the reduction of inflammatory process in mice. She is currently Professor of Food Processing at EARTH University in Costa Rica and works with the processing of some food containing natural additives, without the addition of chemical conservators.

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Marek W Urban

Clemson University, USA

Anisotropic stimuli-responsive polymeric nanoparticles and copolymers with self-healing properties

'his lecture will focus on the design, synthesis and characterization of stimuli-responsive anisotropic nanoparticles with various morphologies. Size- and shape-tunable Janus as well as gibbous and inversegibbous nanoparticles will be discussed in the context of heterogeneous radical polymerization (HRP) developed to synthesize ultra-high molecular weight amphiphilic block copolymers. The second part will describe unique self-healing properties of acrylic-based copolymers which occurs in a narrow compositional range for preferentially alternating with a random component copolymer topology (alternating/random). This behavior is attributed to favorable interchain van der Waals forces forming "key-and-lock" interchain junctions. The use of van der Waals forces instead of supramolecular or covalent rebonding, or encapsulated reactants eliminates chemical and physical alterations and enables multiple recovery upon mechanical damage without external intervention. As a result of perturbation of van der Waals forces resulting from mechanical damage the presence of interdigitated alternating/random copolymer sequences facilitate self-healing under ambient conditions.

Speaker Biography

Marek W Urban is the J.E. Sirrine Foundation Endowed Chair and Professor of Materials Science and Engineering and Chemistry (courtesy) Departments at Clemson University. He received MS in Chemistry from Marquette University, PhD in Chemistry and Chemical Eng. Department from Michigan Technological University, and postdoctoral at Case Western Reserve University. Prior to joining Clemson University, he was a professor, Department Chair and director of polymer science programs at NDSU and USM, where he also directed the Materials Research Science and Engineering (MRSEC) as well as Industry/University Cooperative Research (I/U CRC) Centers funded by the National Science Foundation. He is the author of over 400 research publications and 11 patents, author of four and editor of seven books. His research on self-healing polymers and antimicrobial polymer surfaces has been featured by many media, including NY Times, Forbes, BBC, NBC, Discovery, USA Today, Yahoo, ACS, NSF and many others. He is the Fellow of American Chemical Society PMSE Division, the Royal Society of Chemistry, American Institute of Chemists, and recipient of numerous awards, most recently the Chemical Pioneer Award from Chemical Heritage Foundation (2017) and University Research, Scholarship and Artistic Achievement Award (2018). His research group current research efforts focus on the development of polymeric materials and interfaces with 'living-like' functions. Of recent interests are self-healing commodity polymers, new generations of stimuli-responsive materials with adaptable, sensing, and signaling functions, including colloidal nanoparticles and other nano-objects, as well as spectroscopic imaging methods enabling molecular detection of stimuli-responsiveness.

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Chemistry and Medicinal Chemistry

May 13-14, 2019 | Prague, Czech Republic



Sergey N Fedosov

Aarhus University, Denmark

Transport system of vitamin B12 (Cobalamin) in delivery of therapeutic imaging B12-conjugates: Perspectives and problems

Il animal cells need cobalamin (Cbl, vitamin B12), Abecause Cbl-cofactors are involved in synthesis of DNA and membranes. The uptake of dietary Cbl by humans starts with the binding to a Cbl-specific capturing protein intrinsic factor, which facilitates the intestinal endocytosis. The internalized Cbl is transferred to blood and binds to the specific transporter transcobalamin, which delivers Cbl to all tissues. The specific surface receptor (CD320) renders the cellular uptake of transcobalamin-Cbl, and the endocytosed vitamin is processed to its cofactors via removal of a coordinated inactive group "X" from X- [Co 3+] Cbl. The Cbl-transport system is a vehicle, which guarantees a universal passage through cellular membranes for any compound attached to Cbl, nearly irrespective of its size and chemical features. Yet, modification of Cbl cannot be done at an arbitrary place.

The crystallographic analysis revealed the structural elements, where the attachment of external compounds gives the lowest impact on Cbl-binding. A number of fluorescent and radioactive Cbl-conjugates were used to visualize the main target tissues (e.g. liver, kidney, tumors). Several toxic Cblconjugates with an anti-cancer potential were also described in the literature, but the parallel targeting of both malicious and normal tissues would present a problem for patients. Some alternative approaches are apparently required.

Attachmentofanon-removable "X"-group (in4-ethylphenyl– $[Co^{3+}]$ CbI) demonstrated that such compounds behave as antagonists of CbI, uselessly occupying the CbI-transport

system but giving nearly no gain in the active cofactors. Surprisingly, the tissue accumulation of the unprocessed anti-vitamin was also relatively low, apparently because of a continuous excretion of anti-Cbl from the cells. The overall effect might result in Cbl-exhaustion of the fast propagating cancer cells, combined with a low and revertible impact on other tissues.

Electrochemical synthesis of DNA-Cbl conjugates opened a potential to deliver therapeutic DNAs to the cells *in vivo*. The internalized DNA-Cbl is expected to be split into DNA and Cbl moieties, whereupon the antisense DNA would (i) provoke enzymatic degradation of the target mRNA, and/or (ii) block its translation. Malignant cells have distinct mRNA patterns, implying a possibility of the targeted effect with a low consequence for other tissues. Preliminary work with the "nonsense" DNA-prototypes (suitable for easy tracking) is discussed.

Speaker Biography

Sergey N Fedosov, Aarhus University, worked in different fields of science, covering biochemistry & molecular biology, enzymology & catalysis, organic & inorganic chemistry of cobalamin, synthesis of cobalamin derivatives and adsorbents, computer modeling of metabolism, and medical diagnostics. His work was critical for a number of biotechnological companies, developing pharmacological products. He is known in cobalamin community as inventor of "Fedosov factor" (the combined index of B12 status). He is (co)author of 81 publications), and the overall author-metrics index of h = 28 (Google Scholar).

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Chemistry and Medicinal Chemistry

May 13-14, 2019 | Prague, Czech Republic



Vanya Kurteva

Bulgarian Academy of Sciences, Bulgaria

Chiral anime induced enantioselectivity in trans-β-lactam formation via Staudinger Cycloaddition

A settidine-2-ones, so-called β -lactams, are heterocyclic systems of great importance as they exist as structural subunits in many products of interest as pharmaceuticals, catalysts, synthetic building blocks. The subsequent development of a number of classes of β -lactam antibiotics has made this family of four-membered ring amides one of the most successful classes of therapeutic agents to date. The stereoisomerically pure azetidinones receive special attention as the ring stereochemistry is closely related with their biological activities. Beta-lactam antibiotic families with trans configuration of azetidinone ring, like penems, carbapenems, thienamycines, trinems, cephems, oxacephems, azacephems, etc., have shown extraordinary broad spectrum of activities against aerobic and anaerobic gram-positive and gram-negative organisms.

The stereoselectivity induced during the azetidinone ring construction represents a key element. Despite the diversity of the synthetic protocols developed, the classical Staudinger [2+2] ketene-imine cycloaddition reaction is still of the day and is widely exploited, especially in its asymmetric version by applying chiral auxiliaries. Among the latter, chiral ketene precursors are the most widely applied, while the records in the literature on the efficiency of chiral amines are quite limited. Recently, we reported

on the enantioselective *trans-θ*-lactam synthesis driven by variable commercial chiral amines and showed that the selectivity is strongly dependent both on chiral auxiliary and type, position and number of substituents at aromatic aldehyde unit, i.e. no universal auxiliary is discovered.

This talk will summarize the results on the efficiency of various chiral amines as auxiliaries in the enantioselective construction of *trans-b*-lactam ring via Staudinger cycloaddition.

Speaker Biography

Vanya Kurteva, Prof. Dr. Organic Chemistry, has her expertise in organic synthesis and catalysis. Her team is developed efficient protocols for construction of 2,3-disubstituted imidazo[1,2-a]-pyridines, pirlindole derivatives, N, O-macrocycles, azo-naphthol dyes, etc., as well as various polydentate ligands as synergists and extractants for isolation and separation of metal ions. She spent a research period in the laboratory of Prof. Carlos Afonso (Lisbon, Portugal) working on the synthesis of cyclopentitols, microwave assisted transformations, and reactions in chiral ionic liquids. Her current research interests are focused mainly on the synthesis of procycles with potential interest as chemotherapeutics and ligands for coordination applications. She is a professor and vice-director of the Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences.

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Chemistry and Medicinal Chemistry

May 13-14, 2019 | Prague, Czech Republic



Feng Wang

Swinburne University of Technology, Australia

Decoding isomer fingerprints using Molecular Spectroscopy: Experiment and theory

somers are responsible for biodiversity and bioactivity. Structure dictates properties: An isomer of a potent drug can be toxic. Due to the same composition but different configuration, isomers such as conformers and chiral enantiomers share significant similarities and subtle differences in many properties except for their fingerprint properties. Spectroscopy is a powerful technique to decode fingerprints of isomers when supported by computer powered quantum mechanics. Scientific discoveries in digital age is moving from assisting and analyzing results of spectral characterization to guided designing, controlling and driving experiments with more rational knowledge. Physical properties of almost all materials should be predictable, in principle, by solving the quantum-mechanical equations governing their constituent electrons. This presentation will cover a broach spectrum of theory driven discoveries in molecular spectroscopy at Swinburne University through international collaborations in recent years. In particular, the narrative of collaboration leading to breakthrough of the structure of organometallic compound ferrocene using IR spectroscopy will be presented. I will also report our recent studies using electron momentum spectroscopy (EMS), X-ray photoemission spectroscopy (XPS), nuclear magnetic resonance (NMR) spectroscopy and UV-Vis



spectroscopy to decode the fingerprints of isomers and their intramolecular hydrogen bonding interactions of isomers with biological and pharmaceutical applications. Ferrocene, anticancer drugs, amino acids and other organic compounds such as furfural and tetrahydrofuran etc will be discussed.

Speaker Biography

Feng Wang (PhD Theoretical/Computational Chemistry, Spectroscopy) is Professor of Chemistry and Deputy Chair of Department of Chemistry and Biotechnology at Swinburne University of Technology, Australia. She received her PhD degree at the University of Newcastle (Australia, 1994), worked at the University of Waterloo (1994-1996) as an NSERC Canada International Postdoctoral Fellow and Research Fellow at School of Chemistry, The University of Melbourne (1996-2000). After a short period at a supercomputer centre, she joined Swinburne University of Technology in 2003. She has led many theoretical/ computational chemistry driven discoveries in a broad spectrum of applications in medicinal, biological, solar energy etc in chemistry and physics and has published over 150 peer reviewed journal articles. She is Honorary Professor at School of Chemistry, University of Melbourne, Fellow of RACI and Fellow of the AIP. She also serves on national scientific research committees such as the National Computational Merit Allocation Committee (NCMAC, Australia) and has been an expert panel member for National Research Councils including Ireland, Czech Republic, Portugal, Romania and Canada (Quebec) etc.

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Chemistry and Medicinal Chemistry

May 13-14, 2019 | Prague, Czech Republic



Yasumitsu Matsuo Tomoki Furuseki and Hinako Kawakami

Setsunan University, Japan

Protonics with tissue derived Biomaterials

 ${f B}$ iomaterials are known to be useful in the medical and electrical fields. In the field of energy devices, biomaterials are also attractive materials leading a sustainable society, because these materials are abundant in the natural world and have a potential for the realization of zero emissions. Especially, ion generation and ion transport system with tissue-derived biomaterials are useful for energy sources such as fuel cells. Therefore, research on proton transport based on biomaterials is significantly important to realize a hydrogen energy society in which environmental loads can be responsibly reduced, and thus the investigations of new proton sources and/or new proton-transport materials based on biomaterials are strongly desired. It is known that biomaterials are exhibit proton transport using the mechanism of proton channel, proton pomp and water crosslinking. Recently, we have fabricated bio-based fuel cells using the electrolyte of tissuederived biomaterials such as DNA, collagen and chitin, and we have found that biomaterials can be utilization as the electrolyte of fuel cells. These results indicate that the biomaterial becomes proton conductor. By impedance analyses, collagen, which is one of tissue-derived biomaterials, shows relatively high proton conductivity of 10⁻² S/m in the humidified condition. Further, the power



density in the fuel cell based on collagen electrolyte is approximately $10W/m^2$ and we have found that these biobased fuel cells light the LED. In the present talk, we will show the characteristics feature of bio-based fuel cells based on the electrolyte of tissue-derived biomaterials and will mainly discuss the mechanism on proton conductivity in tissue-derived biomaterials. In addition to these results, we will talk about proton sources based on biomaterials.

Speaker Biography

Yasumitsu Matsuo is a professor in Setsunan University and the chairperson of Department of Life Science in Faculty of Science & Engineering. He has taken a doctorate on science by photoconductivity in GeO₂/Ge bilayer film and thereafter has also investigated the mechanism of proton conductivity in hydrogen-bonded superprotonic conductors. Especially, he has found that superprotonic conductivity in hydrogen-bonded materials is realized by the competition between strain energy and proton kinetic energy including the entropy term. Currently he conductors based on biomaterials. More recently, he has fabricated the fuel cell based on the tissue derived biomaterials and made clear the mechanism of proton conductivity in the humidified biopolymer. In addition, very recently, he has proposed new proton sources using biomaterials and contributes the development of hydrogen energy field as an officer in the Solid-State lonics Society of Japan.

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Chemistry and Medicinal Chemistry

May 13-14, 2019 | Prague, Czech Republic



Yaw-Kuen Li

NCTU, Taiwan

Strategy for constructing antifouling biosensors

iosensors commonly suffer from seriously non-specific Brotein adsorption while measuring real samples in human serum and consequently lead to unreliable responses. To improve the accuracy of detection, biosensor modified with an antifouling surface is indispensable. Though many strategies for reducing non-specific interaction have been developed, the task has not been solved with an acceptable outcome. In particular, after installing the biorecognizers, such as antibodies, for specific targets, the anti-fouling feature of a biosensor is commonly destroyed. How to overcome this problem becomes a main issue of biosensing. We propose and demonstrate an effective protocol via electrodeposition of chargedaniline derivatives for the fabrication of biosensors with promising antifouling ability. The antifouling layer, denoted as (N+S) layer, was constructed on various electrodes via electrodeposition by using the mixture (1:1 molar ratio) of two opposite charged-aniline derivatives, 4-amino-N, N, N-trimethylanilinium (N) and 4-aminobenzenesulfonate (S). In order to know the power of antifouling of (N+S) surface, we compared its cyclic voltammetric property and the feature of human serum adhesion with the

common antifouling surfaces (zwitterionic layers and poly ethylene glycol layers). All the tested surfaces gave similar antifouling power. Yet, the (N+S)-modified surface showed excellent conductivity. The antifouling efficiency of the (N+S) surface is greatly improved with the addition of 1 % sarcosine in human serum as compared with other tested surfaces. On top of the "charged layer", isothiocyanate moieties can be added on with the desired density with which scFvs in the form of proteins or, even better, peptides will be immobilized on the surface of sensor. The standard protocols of screening with phage display library or ribosome display library will be briefly discussed.

Speaker Biography

Yaw-Kuen Li received his PhD degree from Tulane University, USA, in 1991. After his postdoctoral research in School of Medicine of Johns Hopkins University, he moved back to Taiwan to start his academic career in 1993. He was promoted to a full professor in 2002. Further, he became the chair of the department in 2004 and the Dean of college of science in 2014. His primary research interests include three major fields: (a) Enzyme-based catalytic biological reactions, (b) Bio-recognition and Bio-sensors, (c) Solid-state/biological interface chemistry.

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Chemistry and Medicinal Chemistry

May 13-14, 2019 | Prague, Czech Republic



Miguel Holgado

Universidad Politécnica de Madrid, Spain

Arrays of Resonant Nano Pillars (RNPs) for advanced optical biochemical sensing and first steps in tissue-on-a-chip

In recent works we demonstrated the suitability of using resonant nanopillars (R-NPs) arrays for biochemical sensing and label-free biosensing. The performance comparison with other photonic structures suggest the suitability of this transducers and bio-transducers for many other applications. Moreover, the vertical interrogation of the biochips, simplifies the readout platforms and allows a high degree of multiplexing. The multiplexing results showed a highly reproducibility suggesting the potentially of using R-NPs for multiplexed chemical sensors and biosensors. On the other hand, most of the biosensing systems are based on chemical development or amplification (labeled technologies). This is the case of ELISA tests or lateral flow devices. The challenge for label-free PoC devices is to achieve a competitive LoD avoiding this chemical amplification and working with simple drops of samples in an easy-to-use manner. Thus, being the LoD the main figure of merit to compare PoCs, it is worthy to mention that this figure can be improved mainly by enhancing the transducer sensitivity or by reducing the uncertainty of the PoC readout systems. On one hand, the optical transducers employed is decisive for having high sensitivity, and on the other hand, the optical reader (PoCs) is fundamental for readout the signal with low uncertainty and stability. In, fact the LoD can be estimated by the ratio between the uncertainty and the sensitivity and it can be considered the main figure of merit to compare different



biosensing systems. The application of these technologies (transducers and readers) may play an important role in the development of tissue-on-a-chip approaches. We present in this paper the first steps carried out in our research group in tissue-on-a-chip models.

Speaker Biography

Miguel Holgado received his bachelor's and master's degree in Electrical Engineering from Technical University of Madrid (UPM) (1996), and Doctoral degree (Ph.D.) at the Institute of Material Science (ICMM) belonging to the Spanish National Research Council CSIC (2000). He is Deputy Vice-Rector for Innovation, group leader of the Optics, Photonics and Biophotonics at the Center for Biomedical Technology CTB-UPM, and professor at the Applied Physics and Material Engineering Department of Industrial Engineering School (ETSII-UPM). He worked as: R&D engineer at Laser Section at the Spanish Ministry of Defense and responsible for RAMAN spectroscopy service Lab at ICMM-CSIC. He was process engineer at Lucent Technologies Microelectronics for 4 years, Spanish representative in the 5th and 6th European R&D Framework Programme at the Center for Industrial Technology (CDTI), Sub-director of RTD projects at Nanophotonics Technology Center at Technical University of Valencia and Head of European Communities Unit at CSIC. He has led and participated in 34 research projects: 9 European, 19 National and regional as well as another industrial and R&D initiatives. He is author/co- author of more than 150 scientific publications, which have been cited more than 2200 times and the inventor of 6 patents applications. In addition, he is also founder of Bio Optical Detection; a spin-off company (BIOD S.L.) which develops optical Point-of Care devices and offers IVD screening services.

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Chemistry and Medicinal Chemistry

May 13-14, 2019 | Prague, Czech Republic



Jan-Growth Chang

China Medicine University Hospital, Taiwan

Modulating of RNA Alternative Splicing for the treatment of Cancer and Genetic Diseases

NA alternative splicing (AS) is a regulatory mechanism of Regene expression that allows cells to generate more than one mRNA species from a single gene. AS can produce mRNAs which differ in their untranslated regions or coding area through exon skipping, mutually exclusive exons, the use of AS sites, and introns retention. There difference may influence mRNA stability, localization, or translation. AS may contribute to cell differentiation and lineage determination, tissueidentity acquisition and maintenance, and organ development. AS is highly regulated, disturbance of AS machinery leads to mis-splicing, and may result in a range of diseases including cancer, genetic diseases and neurodegenerative disorders. Understanding of the mechanism of AS result in the disease is very important for designing effective therapeutic strategies.

The spatiotemporal changes of AS are governed by combination of cis-regulatory elements and cognate trans-acting factors, which promote or inhibit spliceosome assembly. AS is also controlled by coordinated interactions with other regulatory layers, including transcription and chromatin. Moreover, posttranslational and signaling pathways influence AS through different mechanisms, such as by altering the function and/or localization of key splicing regulators. This extensive crosstalk between gene regulatory layers including dynamic spatial, physical and temporal organizational properties of the cell nucleus, and further emphasizes the importance of developing a multidimensional understanding of AS, and also provides a



theoretical basis of drug design for the treatment of AS-relate diseases and cancer.

To interrogate the treatment of AS-related diseases and cancer, we have developed cell line-system to screen ASmodulating small molecules and using animal model to test their therapeutic effects. More than 500 compounds have been screened, and we found several small molecules have been found to affect the AS of the causing gene of SMA, Fibry's disease, and cancer including modulation of drug resistance. From our results, we suggest that AS-related drugs may affect different layers of AS regulatory machinery, and this effect may influence the therapeutic effect on the diseases. In this talk, I am going to share our previous experience, and present our recent research.

Speaker Biography

Jan-Growth Chang is an expert in the field of molecular diagnosis and treatment of genetic disease and cancer. He was one of the pioneers of the spinal muscular atrophy treatment using small molecules. He was the pioneer to study the diuretic drug-amiloride and its derivatives on RNA alternative splicing and explored their roles at the treatment of cancer and genetic diseases. He has also developed many methods to detect the genetic lesions of genetic diseases and cancer. He is author of over 350 papers and owner of several patents. Now, he is Vice-Superintendent of China Medicine University Hospital, and Director of Department of Laboratory Medicine, Center for Precision Medicine, and Epigenome Research center.

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Chemistry and Medicinal Chemistry

May 13-14, 2019 | Prague, Czech Republic



Jyh-Chiang Jiang

National Taiwan University of Science and Technology, Taiwan

A first-principles study on effects of electric field on heterogeneous catalysis

mproving the selectivity of chemical reactions is arguably the primary challenge in developing an efficient catalyst in catalysis. Electric fields can be used to adjust the thermodynamics of chemical reactions as like temperature and pressure, and it can control selectivity through the field-dipole interactions. Therefore, we attempt to develop an efficient catalyst for the selective methane conversion process and the Iodine reduction reactions as these are essential in solving the environmentally sustainable issues and the energy crises. As indicated in our earlier study, IrO, (110) surface can activate methane at a very low temperature. However, due to the strong reactivity of IrO₂, the adsorbed methane will be completely oxidized, so it is not advantageous to form a value-added chemical on IrO₂. Hence, to adjust the reactivity of IrO₂, here we considered the partial oxidation of methane in the presence of external electric field. Our results demonstrated that we could adjust the adsorption and desorption of the species on the surface with the external electric field. The most favorable reaction pathway is the production of surface formaldehyde by applying a positive external electric field. Likewise, finding and improving the performance of Pt

free counter electrode(CE) in DSSCs is widely researched in energy conversion/storage fields. Hence, here we also investigated the influence of an electric field on the adsorption stability and the possible reduction reactions of I_2 molecule on B-doped, N-doped, B-N co-doped, and pristine graphene nanosheets. Our results show that applying an electric field can significantly enhance the I_2 adsorption and can alter the kinetic properties of the reduction reaction on N-doped graphene under a negative electric field, which will be a potential counter electrode replacement for Pt in DSSC devices. These results demonstrate that the catalytic activity of a catalyst can be effectively controlled by means of the electric field.

Speaker Biography

Jyh-Chiang Jiang graduated from National Taiwan University in 1986 with a B.S. in Chemistry and received his PhD in Chemistry in 1994 from the National Taiwan University. After working as a postdoctoral fellow at IAMS, he joined the faculty of National Taiwan University of Science and Technology (NTUST) in 2001. He has more than 170 papers in peerreviewed journals. His research has also resulted in 4 patents and has been serving as an editorial board member of Scientific Reports.

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Chemistry and Medicinal Chemistry

May 13-14, 2019 | Prague, Czech Republic



J S Sefadi

Sol Plaatje University, South Africa

Clean energy technologies make significant contributions in mitigating the global warming challenges

Energy is the principal resource and most universal measure of all kinds of work by human beings and nature. It is a fundamental contributor in the process of economic, social and industrial development of various hubs around the globe. The traditional energy sources are gradually diminishing, the use of alternative renewable energy sources provide the possible solution to the environment. The significant increase in energy demand is diminishing the non-renewable fossil fuel resources which cause more harm to the environment leading to the most serious global warming challenges. The fundamental ideas of renewable energy resources are related to the issues of sustainability, renewability, pollution and contamination reduction. Hence, the need to discuss various renewable energy resources and their utilization for future growing energy demands. The important development of any country is directly associated to the energy resources present as it is the backbone of energy technology. To mitigate the growing energy demands which continue to create unnecessary pressures on the natural energy resources, it is indispensable for the world to focus on renewable energy technologies to mollify the demand and preserve our finite natural resources for the generations to come. As the primary energy comes from the finite, nonrenewable fossil fuels therefore it's highly crucial to explore other renewable energy possibilities such as biomass, solar, wind, hydroelectric, geothermal, hydrogen gas energy, wave



and tides. This talk will discuss a few options for sustainable energy technologies derived from the organic photovoltaic cells which have a massive industrial application.

Speaker Biography

J S Sefadi is a senior lecturer (Physical Chemistry & materials Science) and an emerging researcher at Sol Plaatje University (SPU). He received his BSc degree in Chemistry Physics (2007); BSc Honours degree in Polymer Science (2008); MSc in Polymer Science (2010) and his PhD degree in Polymer Science (2015) all from University of the Free State. During his spell, he joined the chemistry department at QwaQwa campus as a DST/NRF intern in 2009. He consistently and constantly carried-out the lecturing duties as a junior lecturer in chemistry department for general chemistry, physical chemistry, and inorganic chemistry during the year 2011. He was then appointed as a chemistry lecturer (2014-2015) and then got the green pastures in Kimberley, SPU as senior lecturer, the position he currently holds. He gained an international exposure as a visiting researcher in countries like Solvakia, Bratislava (2009) and Germany, Dresden (2011 & 2012). Upholding an active research status/work with other collaborators, his research interests focus on investigating the renewable and/or sustainable energy projects, climate change etc. He presented his research projects and results at national and international conferences. He has authored publications in scientific peer-reviewed journals and co-authored some scholarly book chapters in SAGE, NOVA and Intech Open Access Publishers. He is currently serving in the Insourcing Advisory Committee (IAC), Institutional Forum (IF), Senate Committee on Research (SCR), Research Chair (RC) and marketing committee of Sol Plaatje University (SPU).

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Chemistry and Medicinal Chemistry

May 13-14, 2019 | Prague, Czech Republic



Feng-Huei Lin

National Health Research Institute, Taiwan

Synthesis and biocompatibility of Diamine biomoleculesfunctinoalized SWCNTs as vectors for Gene Delivery

he development of new and stable gene carrier is of great importance to improve the transfection efficiency and achieve to certain fundamental needs in gene therapy such as therapeutic protein formation, immunogenicity enhancement and apoptosis induction. The stability and applicability of the system that contains single-walled carbon nanotubes (SWNCTs) to combine with plasmid DNA (EGFp-C1) was examine by computer simulation. Raman spectroscopy was used as supporting information to verify the process and phenomenon of complex formation. Two diamine biomolecules, 1,4-diaminobutane and polyoxyethylene bis-amine, were applied in order to load positive charges onto the surface of SWCNTs under physiology condition and also enhance the biocompatibility of SWCNTs. The formation of peptide bond was examined with FTIR spectroscopy to confirm the result of cross liking. Concentration of surface functional groups was examined with TGA, which found that they are at an extremely low concentration but show great influence on the physical property. The binding efficiency of functionalized SWCNTs to EGFp-C1 was analyzed through the binding strength under electrophoresis. Cytotoxicity and cell viability were evaluated with LDH and MTT assay that show a significant

increase in cell viability for SWCNTs-1,4-diaminobuatne complex. The inflammatory inducing property were assessed by pro-inflammatory factor IL-6 release by using quantitative sandwich enzyme immunoassay technique.

Speaker Biography

Feng-Huei Lin is expertise in biomaterials, tissue engineering & regenerative. He obtained his BS degree in Department of Earth Sciences, National Cheng Kung University (NCKU), Taiwan, in 1980. In 1983, he joined the Functional Ceramics Lab in Institute of Materials Sciences and Engineering, NCKU, Taiwan. During the PhD training, he was not only to take course in engineering school, but also in medical school; that included biochemistry, cell biology, physiology, pathology, anatomy etc. He was honored as PhD degree with 12 SCI publications in November 1989. He served as standing committee member in many international societies since 1996. and as editor, associate editor and editorial board members in many SCI journals. He has published over 350 SCI papers, joined 9 book chapters, awarded 78 patents and transferred 27 technologies to industry to be product. He is willing to cooperated with different kinds of researchers and scientists; and very happy to help young blood to do the research by sharing the knowledge, experience and lab tools. He is very experience both in academic research and industry to push the research fruits to the commercial product.

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Chemistry and Medicinal Chemistry

May 13-14, 2019 | Prague, Czech Republic



Bijoy Neog Ankur Gogoi and Nabajyoti Gogoi

Dibrugarh University, India

Role of Garcinia fruits in Obesity control

besity is a global public menace now-a-days, with approximately 315 million people are suffering from this serious health problem. Indigenous herbal medicines may play a very important role in managing obesity as the most of the ailments can be cured through herbal therapy. The complex mixtures of phytochemicals in ethno-medicines often contain that have additive or synergistic interactions. Fruits of Garcinia and unique source of Hydroxycitric acid have a distinct sour taste and has been used for centuries in South-East Asia region to make meals more filling. Inhibition of carbohydrate to fatty acid conversion reaction can lead to obesity control and can be accomplished by assay of Hydroxycitric acid that stops the ATP-citrate lyase formation which is responsible for lipogenesis. (-)-HCA is a derivative of citric acid and found in Garcinia fruits as the principal acid. Our study deals with the subjugating effects of (-)-HCA on lipogenesis in animal model. Wistar rats were fed with a high-fat diet (HFD, 45 kcal% fat) for 60 days. They were given access to food and distilled water ad libitum. The body weights were measured weekly and several important parameters

viz. as Cholesterol, Triglycerides, HDL-D, Cholesterol were recorded. Statistical analyses were performed using SPSS13.Significant changes in body weight between the groups were observed. Supplementation of (-)-HCA significantly lowered visceral fat accumulation in Wistar rats. Our findings establish that Hydroxycitric acid is responsible for repression of lipogenesis in Wistar rats and could be suggested an antiobesity agent.

Speaker Biography

Bijoy Neog has his expertise in Cytogenetics & Plant Breeding. He has worked in biochemical mechanism self-incompatible of Camellia sinensis for his doctoral thesis. He has keen interest in multidisciplinary approaches in biological sciences and has authored of over 50 research papers and book chapters in various National and International Journals. His special interest is in the field of lesser known fruit species of pharmaceutical importance from eastern Himalayan Region of Indo-China Border. He was awarded prestigious Chinese Government Scholarship for Post-Doctoral Research in 2005-06. He has P.G.teaching experience for 24 years and presently working as Professor in the Department of Life Sciences, Dibrugarh University, Assam, India.

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Chemistry and Medicinal Chemistry

May 13-14, 2019 | Prague, Czech Republic



Yuh-Lin Wang

National Taiwan University, Taiwan

Rapid bacterial antibiotic susceptibility tests based on Simple Surface-Enhanced-Raman Spectroscopic Biomarkers

Rapid bacterial antibiotic susceptibility tests (AST) Pare important to help reduce the mortality of sepsis patients, the widespread misuse of antibiotics and the growing drug-resistance problem. We discovered that, when a susceptible strain of bacteria is exposed to an antibiotic, the intensity of specific biomarkers in its surface enhanced Raman scattering (SERS) spectra drops evidently in two hours. The discovery has been exploited for rapid antibiotic susceptibility test (AST) – dubbed SERS-AST, of bacteria cultured from the blood samples of sepsis patients. By applying 3~4 antibiotics to every clinical sample, a total of more than six hundred cases of SERS-AST was conducted; and the overall successful rate of identifying the bacteria's antibiotic susceptibility was 95.7%.

The biomolecules responsible for these bacterial SERS biomarkers have been identified as several purine derivative metabolites involved in bacterial purine salvage pathways. Using ultra-performance liquid chromatography/ electrospray ionization-mass spectrometry (UPLC/ESI-MS),

the time dependences of the concentrations of these molecules were measured. Surprisingly, a single S. *aureus* and E. *coli* cell were found to release millions of adenine and hypoxanthine into a water environment in an hour respectively. The implications of these findings about the molecular origin of the SERS biomarkers to the emergent SERS-AST method will be addressed in conjunction with other emergent AST methods.

Speaker Biography

Yuh-Lin Wang, Dr. Physics, specializes in the creation and applications of novel nanostructures that are formed solid surfaces via constrained self-organization processes. He is a co-author of more than 150 papers and the recipient of several awards including the Prime Minister Award for Outstanding Contribution in Science and Technology, Taiwan and Academic Award, Ministry of Education, Taiwan. He is a fellow of American Physical Society, U.S.A. He is an adjunct professor of the department of physics, National Taiwan University, Taiwan.

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